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Temperature Mapping with STEM Atomic Scale Debye-Waller Thermometry

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With the miniature of electronics, thermal interface resistance (TIR) becomes one of the crucial factors limiting the scalability of integrated circuits, and further dictating the performance of devices. Technique that can measure temperature (*T*) gradient with high spatial resolution and precision is in demand to understand TIR. Existing thermometry techniques, such as Raman spectroscopy, time-domain thermo-reflectance and scanning thermal microscopy, are limited by the wavelength or physical size of the probe and only can achieve ~100 nanometers resolution [1]. (Scanning) transmission electron microscopy [(S)TEM] can be promising in this regard due to the short wavelength of electrons. Non-contact temperature mapping has been explored in STEM including binary thermometry utilizing phase change [2], thermal strain mapping by electron energy loss spectroscopy [3] and diffraction analysis [4], which achieves ~10 nanometer spatial resolution. Here, we report the novel STEM thermometry based on quantifying Debye-Waller effect from atomic resolution imaging, which is coined Debye-Waller (DW) thermometry. Our method has the benefits of high spatial resolution, precise temperature quantification, simultaneous structure characterization and easy implementation [5]. We will also report the application of DW thermometry to map the temperature profile across the FIB-prepared GaN device.

Atoms vibrates collectively in material due to thermal energy. Such motion, namely phonons, can greatly influence the trajectory of electrons and in turn affect the (S)TEM signals, which is known as DW effect. Therefore, *T* can be measured using STEM by quantifying the DW effect. However, precise understanding of the scattering behavior of electrons with respect to materials' *T* is required to realize such capability. In this study, we report the sensitivity of electron scattering to *T* as a function of the scattering angle in in situ STEM. The scattering intensities at higher angle ranges are known to be dominated by thermal diffuse scattering and expected to decrease with increasing temperature because of disrupted channeling conditions. On the other hand, temperature sensitivity of the intensities at lower scattering angles is less understood. Taking advantage of high dynamic range pixelated detector and sub-Ångstrom electron probe, 2D diffraction patterns are collected as a function of 2D real space scanning array, namely 4D-STEM. The 4D-STEM dataset is first spatially averaged to generate the position averaged convergent beam electron diffraction (PACBED) pattern (Fig. 1a). By comparing the azimuthally averaged intensity of PACBEDs collected at different temperatures (Fig. 1b), we demonstrate that the scattering intensities at low-to-intermediate angles increase at higher *T*, which is opposite to the behavior at higher angles (Fig. 1c and 1d). The amplitude of the change is also larger than that in high angle scattering. We then advance the study to even higher resolution by analyzing the temperature susceptivity of column intensities of atomic resolution images reconstructed from 4D-STEM dataset as a function of collection angles (Fig. 2a-c). Similarly, the images formed with electrons scattered to low-to-intermediate angles show increasing column intensity at higher temperature but opposite trend for the ones formed with electrons scattered to higher angle. The observations provide the possibility to probe temperature at unit cell resolution with PACBED pattern matching or even atomic resolution by quantifying intensity change of atomic columns.

Next, we demonstrate the capability of DW thermometry to map *T* of a house-made device. A hole is trenched next to the heating coil of a commercially available DENs chip to create an out-of-equilibrium thermal condition. A FIB-prepared GaN lamella is used to bridge the heat source with the heat sink, and a *T* gradient is expected to form along the direction of the heat flow. By collecting atomic resolution images from numerous regions and analyze the change in column intensity, we successfully map the *T* profile as shown in Fig. 3d-h. Our result promises the further understanding of TIR by providing a novel method that can measure structure and *T* simultaneously with high spatial resolution and precision [6].

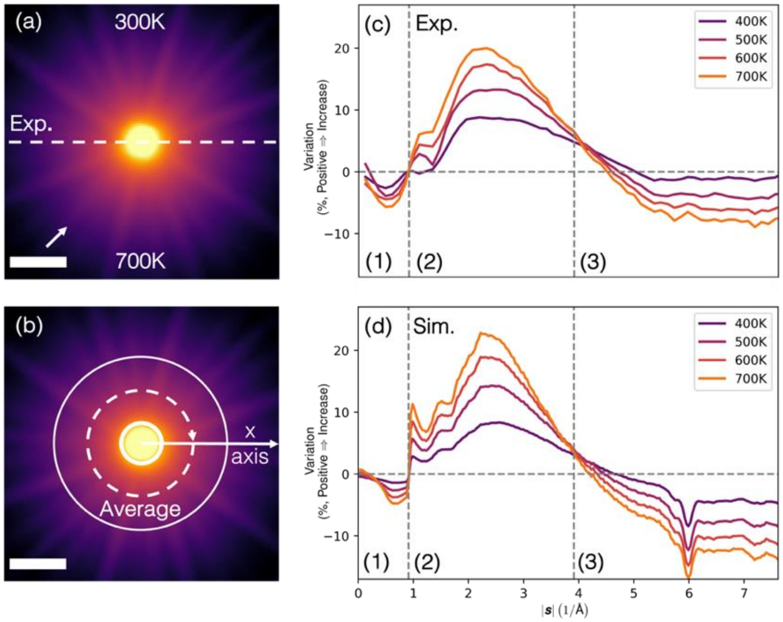

Figure 1 (a) Experimental PACBED collected under 300 (top half) and 700K (bottom half). Arrow indicates the location of HOLZ line. (b) PACBED patterns are annularly averaged as a function of scattering angle as shown in the schematic to get line profiles. (c) Experimental line profiles under different temperatures are normalized with respect to the one under 300K and the percentage variation is shown as a function of scattering angle. Two inversions are indicated by vertical dashed lines. Positive values indicate intensity increases at given temperature. (d) Simulated counterpart of (c).

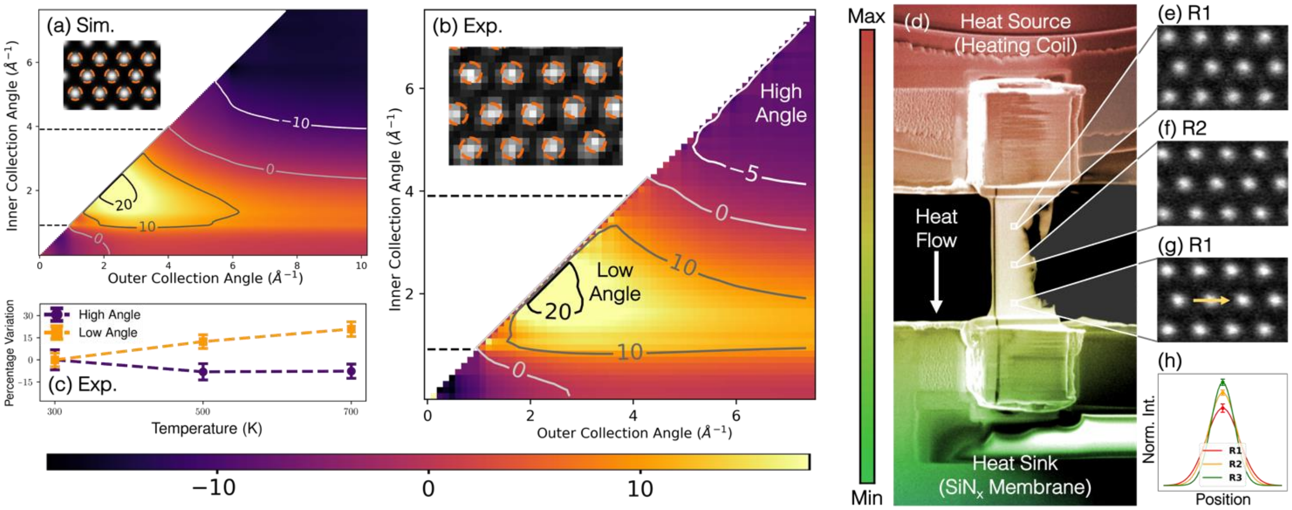

Figure 2 (a) The inset shows one representative image reconstructed from simulated 4D-STEM data. Such images are reconstructed as a function of inner and outer collection angle at 300 and 700 K, respectively. The intensity variation of the orange circled column is taken between 700 and 300 K and plotted in (a). The two horizontal dashed lines indicate the location where inversion/crossover happens. (b) Experimental counterpart of (a). (c) Images are reconstructed from experimental 4D-STEM data with $1.9 - 2.6$ Å^{-1} (low angle) and $5.9 - 7.1$ Å^{-1} (high angle) collection angle for 300, 500, and 700 K. The collection angles are labeled in (b). The percentage variation of column intensity with respect to 300 K is plotted as a function of *T*. The error bar indicates the standard deviation propagating from the non-uniform intensities measured from numerous columns. The color bar at the bottom applies to (a) and (b). (d) Temperature map of a house made GaN device. By trenching a hole on commercial DENs heating chip, heat flow is generated from the heat source to the heat sink. Temperatures from numerous 20 by 20 nm regions are probed with method shown in Figure 2a-c, and the rest of the map were generated by interpolation. (e)-(g) Representative atomic resolution images from three probed regions. (h) Averaged intensity line profiles from R1-R3 across the atomic column [arrow shown in (g)].

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